

## **Quick Theta/2-Theta Measurement (BB) Part**



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## 1. How to set Part conditions

In this chapter, how to set the **Quick Theta/2-Theta Measurement (BB)** Part conditions is described.

### 1.1 Setting conditions

Set the basic conditions in the **Quick Theta/2-Theta Meas. (BB)** dialog box.

The scan conditions and slit conditions of the quick theta/2-theta measurement are determined based on the basic conditions. The scan conditions and slit conditions can also be customized.

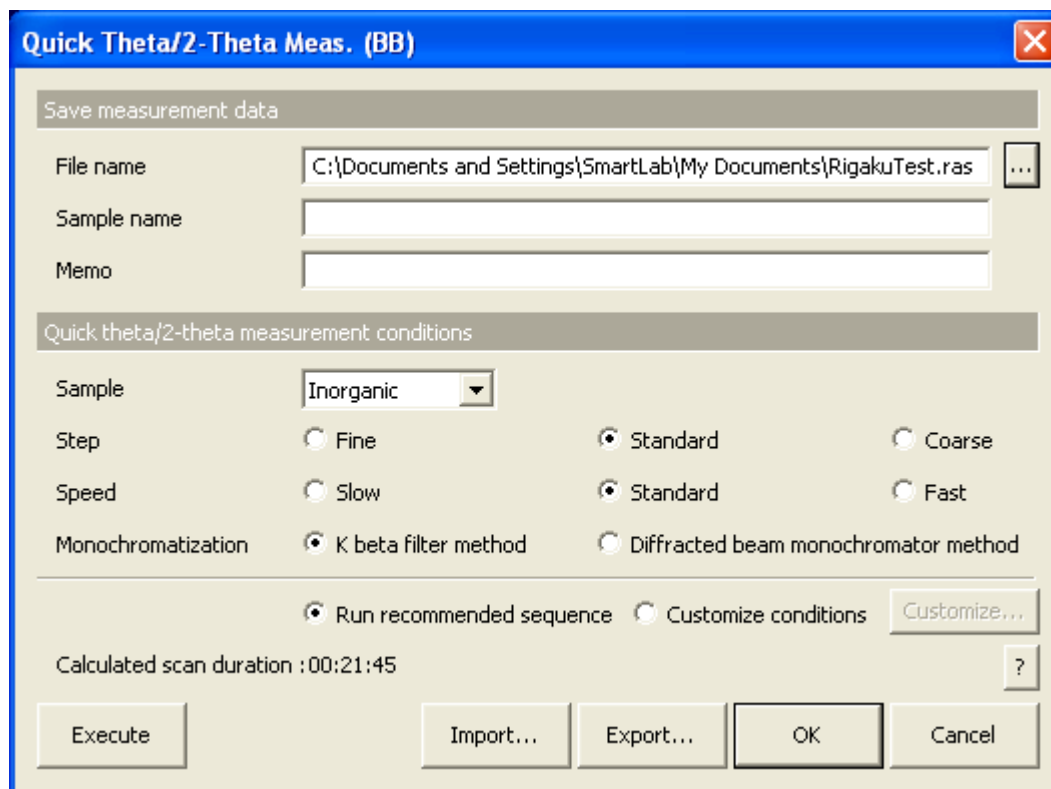


Fig. 1.1.1 Quick Theta/2-Theta Meas. (BB) dialog box

- File name** Enter the name of the file to save the measurement data in.
- Sample name** Enter the sample name (optional). The sample name entered here will be saved in the measurement data file.
- Memo** Enter the memo (optional). The memo entered here will be saved in the measurement data file.
- Sample** Select the type of sample to be measured from **Inorganic**, **Organic**, **Mineral**, or **Metal**. If the sample is a mixture of different material types or the material of the sample is unknown, select **Unknown**.

**Step** Select the step width of the scan from **Fine**, **Standard**, or **Coarse**. In ordinary cases, select **Standard**.

Fine	Select <b>Fine</b> if the step width is suspected to be narrower than the FWHM (0.1°) of ordinary diffracted beams.
Standard	Sets the step width to 1/5 of the FWHM (0.1°) of ordinary diffracted beams.
Coarse	Select <b>Coarse</b> if the step width is suspected to be wider than the FWHM (0.1°) of ordinary diffracted beams.

**Speed** Select the scan speed from **Slow**, **Standard**, or **Fast**. In ordinary cases, select **Standard**.

Slow	Select <b>Slow</b> if you wish to improve the quality of the measurement data. However, measurement duration will be longer.
Standard	Measurement duration will be 15 to 30 minutes. The data thus obtained should cause no problems in the phase ID analysis of an ordinary sample.
Fast	Select <b>Fast</b> if you wish to shorten measurement duration. However, the quality of the measurement data will be lower.

**Monochromatization** Select from **K beta filter method** or **Diffracted beam monochromator method**.

K beta filter method	This method removes almost all $K\beta$ x-rays only by inserting the metal filter into the x-ray path ( $K\alpha : K\beta = 100 : 1$ ). If the DBM unit is not available or it is annoying to exchange the optical devices, select this method.
Diffracted beam monochromator method	If the DBM unit (option) is available, it is recommended to select this method. The diffracted beam monochromator method is to monochromatize x-rays using the diffraction by a crystal. This setting removes almost all x-rays ( $K\beta$ x-rays, continuous x-rays, fluorescent x-rays, etc.) other than those of the selected wavelength and provides measurement data with a low background level.

**Run recommended sequence** Makes the quick theta/2-theta measurement using the recommended sequence.

**Customize conditions** Makes the quick theta/2-theta measurement under the conditions specified in the **Customize** dialog box.

**Customize**

When the **Customize conditions** radio button is selected, click the **Customize** button, then set the scan conditions and slit conditions.

 [エラー! 参照元が見つかりません。](#)

**Calculated scan duration**

Shows the calculated duration of the quick theta/2-theta measurement.

**Execute**


Executes the quick theta/2-theta measurement under the conditions specified in the **Quick Theta/2-Theta Meas. (BB)** dialog box.



**CAUTION:** Clicking the **Cancel** button after executing the quick theta/2-theta measurement does not cancel the specified conditions.



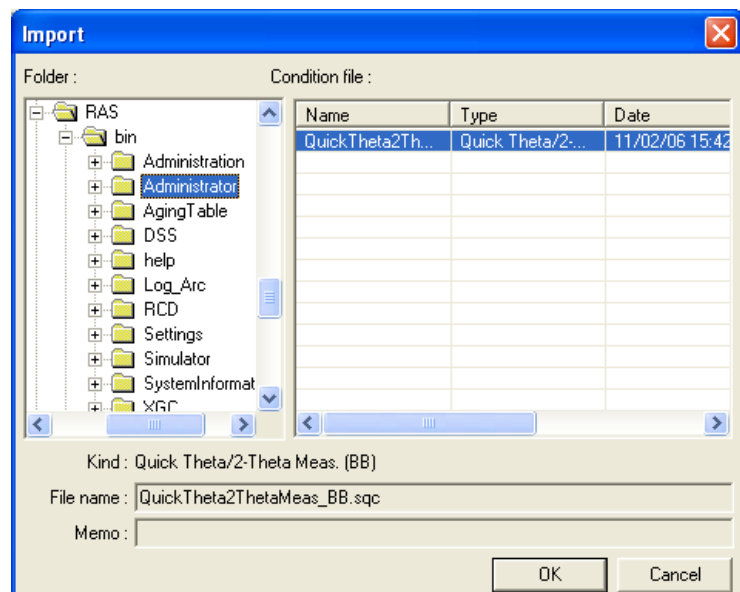
**Tip:** The quick theta/2-theta measurement is executed with the **Quick Theta/2-Theta Meas. (BB)** dialog box open. While the quick theta/2-theta measurement is running, the Part conditions cannot be changed. They can be changed again after the measurement has been completed.

The setting of  (Show confirmation messages) on the flow bar becomes invalid.

**Import**

Loads the saved Part conditions.

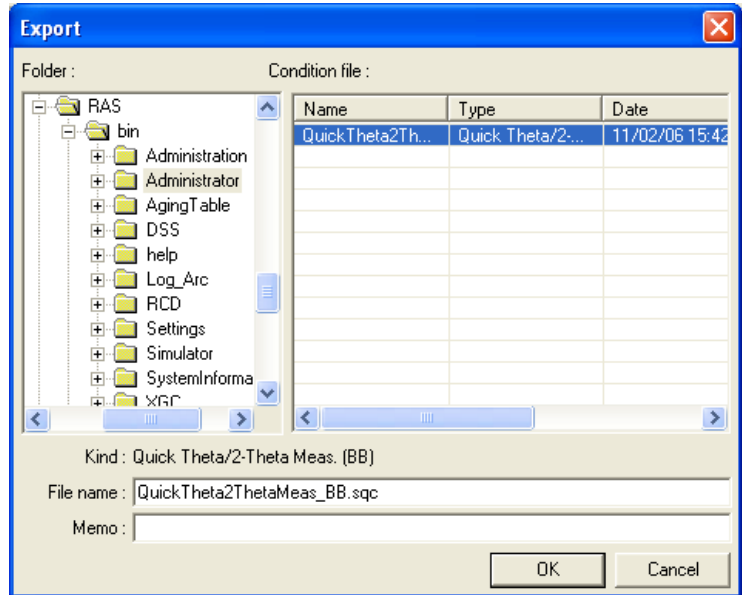
Clicking the **Import** button opens the **Import** dialog box. Select the folder including the file you want to import from the **Folder** tree view. In the **Condition file** list, select the condition file you want to import and click the **OK** button to load the Part conditions.



### Export

Saves the specified Part conditions in a file.

Clicking the **Export** button opens the **Export** dialog box. From the **Folder** tree view, select a destination folder to save the conditions file then enter a file name in the **File name** box. Enter comments in the **Memo** box, if needed. After entering them, click the **OK** button.



### OK

Sets the conditions and closes the dialog box.



**CAUTION:** When selecting another Package measurement or switching the task to the **Manual Control** task, etc. the specified conditions will be cancelled. To save the specified conditions in a file, click the **Export** button and save the conditions.

### Cancel

Does not set the conditions and closes the dialog box.



**Tip:** Clicking the **Cancel** button also cancels the conditions specified in the **Customize** dialog box.

### ?

Opens the online help of this Part.



## 1.2 Customizing scan conditions and slit conditions

If you want to customize the scan conditions and slit conditions of the quick theta/2-theta measurement, set the conditions in the **Customize** dialog box.



Tip: Refer to [2. Measurement sequence](#) to set the scan conditions and slit conditions.

**Customize - Quick Theta/2-Theta Meas. (BB)**

Quick theta/2-theta measurement conditions

Sample:

Step:  Fine  Standard  Coarse

Speed:  Slow  Standard  Fast

Monochromatization:  K beta filter method  Diffracted beam monochromator method

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Slit conditions

Soller/PSC (deg)	IS (deg)	IS L (mm)	R51 (deg)	PSA (deg)	Soller (deg)	R52 (mm)	IS (mm)	R51 (mm)	R52 (mm)
5.0	2/3	10.0	2/3	Open	5.0	0.300	2.211	1.315	0.300

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Measurement conditions

Scan axis	Mode	Range	Start (deg)	Stop (deg)	Step (deg)	Speed (deg/min)	Attenuator	Comment
Theta/2-Theta	Continuous	Absolute	3.0000	90.0000	0.0200	4.0000	Open	0.0000

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Oscillation/Rotation

Exec.	Axis	Action	Range	Origin(Center) (deg)	Oscillation range (+/-) (deg)	Start (deg)	Stop (deg)	Speed (deg/min)
<input checked="" type="checkbox"/>	Chi	Oscillation	Absolute	0.000	1.000	0.000	10.000	5
<input type="checkbox"/>	Phi	Oscillation	Absolute	0.000	1.000	0.000	1.000	5
<input type="checkbox"/>								

Calculated scan duration : 00:21:45

**Fig. 1.2.1** Customize dialog box

Quick theta/2-theta measurement conditions

Sample:

Step:  Fine  Standard  Coarse

Speed:  Slow  Standard  Fast

Monochromatization:  K beta filter method  Diffracted beam monochromator method

### Sample

Select the type of sample to be measured from **Inorganic**, **Organic**, **Mineral**, or **Metal**. If the sample is a mixture of different material types or the material of the sample is unknown, select **Unknown**.

**Step**

Select the step width of the scan from **Fine**, **Standard**, or **Coarse**. In ordinary cases, select **Standard**.

Fine	Select <b>Fine</b> if the step width is suspected to be narrower than the FWHM (0.1°) of ordinary diffracted beams.
Standard	Sets the step width to 1/5 of the FWHM (0.1°) of ordinary diffracted beams.
Coarse	Select <b>Coarse</b> if the step width is suspected to be wider than the FWHM (0.1°) of ordinary diffracted beams.

**Speed**

Select the scan speed from **Slow**, **Standard**, or **Fast**. In ordinary cases, select **Standard**.

Slow	Select <b>Slow</b> if you wish to improve the quality of the measurement data. However, measurement duration will be longer.
Standard	Measurement duration will be 15 to 30 minutes. The data thus obtained should cause no problems in the phase ID analysis of an ordinary sample.
Fast	Select <b>Fast</b> if you wish to shorten measurement duration. However, the quality of the measurement data will be lower.

**Monochromatization**

Select from **K beta filter method** or **Diffracted beam monochromator method**.

K beta filter method	This method removes almost all $K\beta$ x-rays only by inserting the metal filter into the x-ray path ( $K\alpha : K\beta = 100 : 1$ ). If the DBM unit is not available or it is annoying to exchange the optical devices, select this method.
Diffracted beam monochromator method	If the DBM unit (option) is available, it is recommended to select this method. The diffracted beam monochromator method is to monochromatize x-rays using the diffraction by a crystal. This setting removes almost all x-rays ( $K\beta$ x-rays, continuous x-rays, fluorescent x-rays, etc.) other than those of the selected wavelength and provides measurement data with a low background level.



Tip: When the **Close** button is clicked after setting four conditions in the **Quick theta/2-theta measurement conditions** section in the **Customize** dialog box, the conditions in the **Quick Theta/2-Theta Meas. (BB)** dialog box will also be changed.

Slit conditions									
Soller/PSC (deg)	IS (deg)	IS L (mm)	RS1 (deg)	PSA (deg)	Soller (deg)	RS2 (mm)	IS (mm)	RS1 (mm)	RS2 (mm)
5.0	2/3	10.0	2/3	Open	5.0	0.300	2.211	1.315	0.300

Table 1.2.1 shows the choices of the widths or lengths of the slits and the aperture angles of the parallel slits.

<b>Soller/PSC (deg)</b>	Select the aperture angle of the incident parallel slit.
<b>IS (deg)</b>	Select or enter the width of the incident slit. The value entered here is shown in the <b>IS (mm)</b> box in terms of mm.
<b>IS L (mm)</b>	Select the length of the length limiting slit.
<b>RS1 (deg)</b>	Select or enter the width of the receiving slit # 1. The value entered here is shown in the <b>RS1 (mm)</b> box in terms of mm.
<b>PSA (deg)</b>	Select the aperture angle of the PSA.
<b>Soller (deg)</b>	Select the aperture angle of the receiving parallel slit.
<b>RS2 (mm)</b>	Select or enter the width of the receiving slit # 2.



Tip: The slit width can be entered in fractional number such as “1/2”, “2/3”.

**Table 1.2.1 Choices of the width, length, or aperture angle of each slit**

Slit	Width, length, or aperture angle
Soller/PSC (deg)	5.0, 2.5, 1.0, 0.5, 0.15, Open
IS (deg)	2/3, 1/2, 1/3, 1/4, 1/6, 1/8, Open
IS length limiting slit (mm)	15.0, 10.0, 5.0, 2.0, 0.5, None
RS1 (deg)	2/3, 1/2, 1/3, 1/4, 1/6, 1/8, Open
PSA (deg)	1.0, 0.5, 0.114, Open, None, No_unit
Soller (deg)	5.0, 2.5, 1.0, 0.5, 0.114, None, No_unit
RS2 (mm)	0.60, 0.45, 0.3, 0.15, 0.10, 0.05, Open

## 1. How to set Part conditions

Measurement conditions									
Scan axis	Mode	Range	Start (deg)	Stop (deg)	Step (deg)	Speed (deg/min)	Attenuator	Comment	
Theta/2-Theta	Continuous	Absolute	3.0000	90.0000	0.0200	4.0000	Open	0.0000	

**Scan axis** Select the scan axis from **Theta/2-Theta**, **2-Theta**, **Omega**, or **2-Theta/Omega**.

**Mode** Select the scan mode from **Continuous** or **Step**.

**Start (deg)** Enter the start angle of the scan.

**Stop (deg)** Enter the stop angle of the scan.

**Step (deg)** Enter the step width of the scan.

**Speed (deg/min) / Duration time (sec)**

When **Continuous** is selected as the scan mode, enter the scan speed. When **Step** is selected as the scan mode, enter the duration time per measurement point.

**Attenuator** Select the attenuator to be used for the data measurement from **Open**, **1/70**, **1/1000**, or **1/10000**.

**Omega (deg) / 2-Theta (deg) / delta Omega (deg)**

When **2-Theta** or **Omega** is selected for **Scan axis**, enter the position of the omega or 2-theta axis, respectively. When **2-Theta/Omega** is selected for **Scan axis**, enter the offset angle of the omega axis.



Tip: When **2-Theta/Omega** is selected for **Scan axis**, the range of the omega axis is given by the following equations:

start angle: (value entered in the **Start (deg)** box) / 2 + **delta Omega**

stop angle: (value entered in the **Stop (deg)** box) / 2 + **delta Omega**

**Comment** Enter the comment (optional). The comment entered here will be saved in the measurement data file.

Oscillation/Rotation								
Exec.	Axis	Action	Range	Origin(Center) (deg)	Oscillation range (+/-) (deg)	Start (deg)	Stop (deg)	Speed (deg/min)
<input checked="" type="checkbox"/>	Chi	Oscillation	Absolute	0.000	1.000	0.000	10.000	5
<input type="checkbox"/>	Phi	Oscillation	Absolute	0.000	1.000	0.000	10.000	5
<input type="checkbox"/>								

**Exec.** When the **Exec.** box is checked, the selected axis will be oscillating or spinning during the measurement.

**Axis** Select the axis to oscillate or spin.

**Action** Select the action of the selected axis from **Oscillation** or **Spin**.



Tip: The available actions depend on the selected axis.

**Range** When **Oscillation** is selected as the action of the selected axis, select **Absolute** or **Relative** as the oscillation range specification method.

**Origin (center)(deg)** When **Oscillation** is selected as the action of the selected axis and **Relative** is selected as the oscillation range specification method, enter the oscillation center.

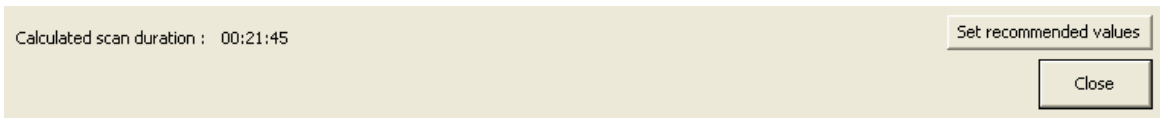
**Oscillation range (+/-)(deg)** When **Oscillation** is selected as the action of the selected axis and **Relative** is selected as the oscillation range specification method, enter the oscillation width.

**Start (deg)** When **Oscillation** is selected as the action of the selected axis and **Absolute** is selected as the oscillation range specification method, enter the oscillation start angle.

**Stop (deg)** When **Oscillation** is selected as the action of the selected axis and **Absolute** is selected as the oscillation range specification method, enter the oscillation stop angle.

**Speed (deg/min)** Enter the oscillation or spin speed.

**1. How to set Part conditions**



- Calculated scan duration** Shows the calculated duration of the quick theta/2-theta measurement.
- Set recommended values** Sets the conditions in the **Slit conditions** and **Measurement conditions** sections to the recommended values based on the conditions specified for **Sample**, **Step**, and **Speed**. The recommended values are shown in Tables 1.2.2 and 1.2.3.
- Close** Closes the **Customize** dialog box.

**Table 1.2.2 Recommended slit conditions**

Sample	Soller/PSC	IS	IS L	RS1	PSA	Soller	RS2
Inorganic	5 deg	2/3 deg	10 mm	2/3 deg	Open	5 deg	0.3 mm
Organic		1/3 deg		1/3 deg			
Mineral		1/3 deg		1/3 deg			
Metal		2/3 deg		2/3 deg			
Unknown		1/3 deg		1/3 deg			

**Table 1.2.3 Recommended measurement conditions**

Sample	Scan axis	Mode	Start	Stop	Step	Speed	Attenuator	Omega / 2-Theta / delta Omega
Inorganic	Theta/ 2-Theta	Conti-nuous	3 deg	90 deg	0.01 deg (Fine)	1 deg/min (Slow)	Open	0 deg
Organic			2 deg	60 deg	0.02 deg (Standard)	4 deg/min (Standard)		
Mineral			2 deg	70 deg		8 deg/min (Fast)		
Metal			5 deg	120 deg		0.04 deg (Coarse)		
Unknown			2 deg	90 deg				

## 2. Measurement sequence

The quick theta/2-theta measurement is performed automatically. However, the length limiting slit, parallel slit, etc. must be installed (or removed) manually as instructed by messages displayed on the screen.

Described below is the general measurement sequence.

- (1) When **K beta filter method** is selected as the monochromatization method, insert the K $\beta$  filter for Cu into the receiving slit box # 1, and install the scintillation counter onto the counter adaptor as instructed by the message.

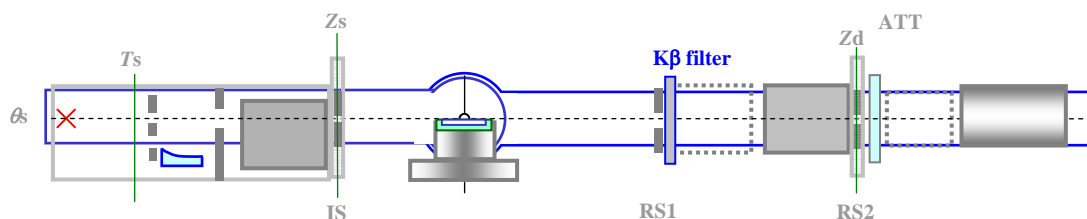


Fig. 2.1 Monochromatization (K beta filter method)

When **Diffracted beam monochromator method** is selected as the monochromatization method, install the DBM unit (Bent) onto the counter adaptor as instructed by the message.

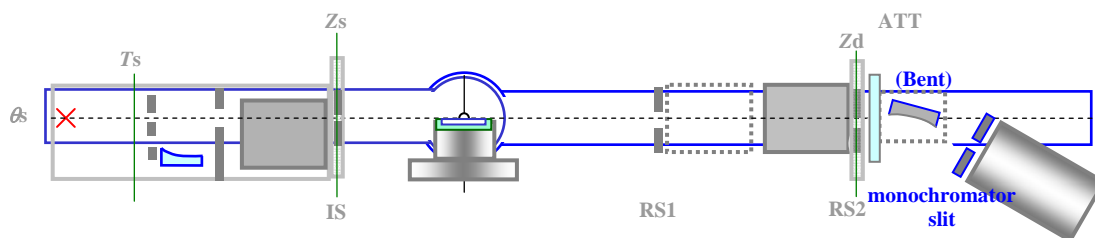
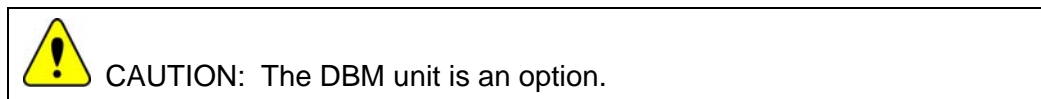


Fig. 2.2 Monochromatization (diffracted beam monochromator method)

- (2) Make the data measurement under the conditions specified in the **Quick Theta/2-Theta Meas. (BB)** dialog box.

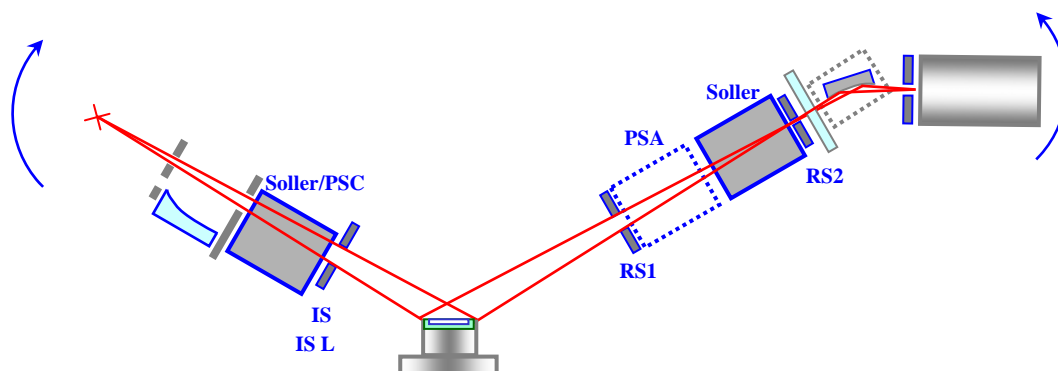


Fig. 2.3 Theta/2-theta measurement using the DBM unit